

Oxazole
288-42-6 | DTXSID70182983

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.30e-01

Global applicability domain: Inside

Local applicability domain index: 4.96e-01

Confidence level: 7.63e-01

Nearest Neighbors from the Training Set

Image not found

Oxazole

Measured: 0.12

Predicted: 2.30e-01

Image not found

Isoxazole

Measured: 0.08

Predicted: 3.62e-01

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Imidazole

Measured: -0.0800

Predicted: -0.238

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2-Methoxyfuran

Measured: 1.44

Predicted: 1.30

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Pyrazine

Measured: -0.260

Predicted: 8.12e-02